

Isonipecotic acid, n-butoxycarbonyl-, isohexyl ester

Inchi: InChI=1S/C17H31NO4/c1-4-5-12-22-17(20)18-10-8-15(9-11-18)16(19)21-13-6-7-14(2)3/
InchiKey: DNKBPBFVYXZEJW-UHFFFAOYSA-N
Formula: C17H31NO4
SMILES: CCCOC(=O)N1CCC(C(=O)OCCCC(C)C)CC1
Mol. weight [g/mol]: 313.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.62		Crippen Method
logp	3.614		Crippen Method
mcvol	264.390	ml/mol	McGowan Method
rinpol	2228.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U322050&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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